n-Hexane
110-54-3 | DTXSID0021917

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 211 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

Image not found
Ethylbenzene
Measured: 170
Predicted: 271

Image not found
Styrene
Measured: 912
Predicted: 358

Image not found
para-Xylene
Measured: 257
Predicted: 246

Image not found
Toluene
Measured: 117
Predicted: 87.4

Image not found
4-Methylaniline
Measured: 79.4
Predicted: 104